ADVANCED CHEMISTRY BASINS MODEL TECHNICAL REPORT

- Covering the period from June 11, 2001 – Dec 3, 2001

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- Issued December, 2001

EXECUTIVE SUMMARY

The advanced Chemistry Basin Model project has been operative for 30 months. During this period, most project tasks are on projected schedule (up to 150% of goals). On average the project is on schedule (100%). The goal of the past 6 months has been to add functionality to the prototype described in the last semi-annual report.

MILESTONE SCHEDULE/STATUS

The only milestone listed in the project is to have a prototype model operational on a workstation. Progress towards that goal has been substantial (as detailed below) and on schedule. In conformance with good software design requirements, the prototype has been designed modularly, in several pieces. Each of the pieces has been tested independently. With such a design, testing communications between the pieces becomes problematic, as the pieces are only weakly-coupled. However, this potential pitfall has been overcome, and several code modules have been successfully combined during the reporting period. The prototype has achieved 'alpha' stage: it is running, but significant bugs still exist, and much additional functionality remains to be added. The goals for the next year include moving the model to beta stage (where all functionality is present, though significant bugs still exist), developing documentation, and preparing a distribution. What remains is to then incorporate all scientific results in the prototype, debug it, and improve usability.

TASK 1: MATURITY INDICATORS

Primary Responsibility	Current Subtasks	Investigator
Caltech	Develop algorithms	Tang

Summary: The first task is to "Develop a database of additional and better maturity indicators for paleo-heat flow calibration". Fundamental to this development is to perform a series of controlled kinetic experiments on maturity indicator evolution. The third year subtask is to "Study the vitrinite reflectance suppression.[1] Comparing different thermal indicators and testing them under geological conditions. Establish the complete database for worldwide vitrinite reflectance kinetics".

Significant efforts are currently focused on (1) maturity effects by different degrees of biodegradation, and (2) high temperature maturity parameters. For biodegradation, we have looked at heavily biodegraded crude oils of the San Joaquin Valley, California. All biomarker parameters have been quantified, completed ahead of schedule. These quantifications are being incorporated in the model under Task 6.

TASK 2: COMPOSITIONAL MATURATION

Primary Responsibility	Subtask	Investigator
Caltech	Establish a reaction network	Tang

Summary: The second task is to "Develop maturation models capable of predicting the chemical composition of hydrocarbons produced by a specific kerogen as a function of maturity, heating rate, etc.; assemble a compositional kinetic database of representative kerogens." For the third year of the project, the sub-task is to "Add additional generation models with kinetic parameters describing the breakdown of a typical range of kerogens. Analyze additional pyrolysis experiments to derive the needed parameters."

We are working on the quantitative analysis of our open system time resolved compositional pyrolysis GC. Two kerogen samples have been used as testing samples: a Green River shale sample and a Green River Coal sample. The main efforts are to improve the high molecular weight waxy components. For the oil cracking experiment, we are running a comparison study between oil cracking under water and anhydrous cracking to isolate water and clay effects.

We have also continued development on the technology to decouple gas generation from primary kerogen cracking and secondary oil cracking process. Among the systems to be studied include Cameo coal, Kimmeridge shale, Brown limestone, and other typical source rocks.

TASK 3: EQUATION OF STATE FLASH CALCULATION

Primary Responsibility	*Subtask*	*Investigator*
Caltech	EOS model	Meulbroek

Summary: The third task of the project is to "Develop a 4 phase equation of state-flash model that can define the physical properties (viscosity, density, etc.) of the products of kerogen maturation, and phase transitions that occur along secondary migration pathways." For the third year of the project, the sub-task is to: "refine and verify component class divisions."

Current work includes (1) expanding the 2-phase model developed in the past 6 months to 3-phases, (2) developing predictive models for viscosity. Future goals include developing a solid-phase equilibrium model to predict wax and asphaltene deposition.

The past 6 months have seen the final incorporation of the two-phase model into the prototype basin model using COM technology. The code developed in perl during the last reporting period was successfully incorporated into the prototype this period. The use of COM technology also allows these sections of the software package to be run stand-alone, allowing greater utility. To demonstrate this technology, a MS Excel prototype was assembled that incorporates the flash model. A screen shot of that model is shown below.
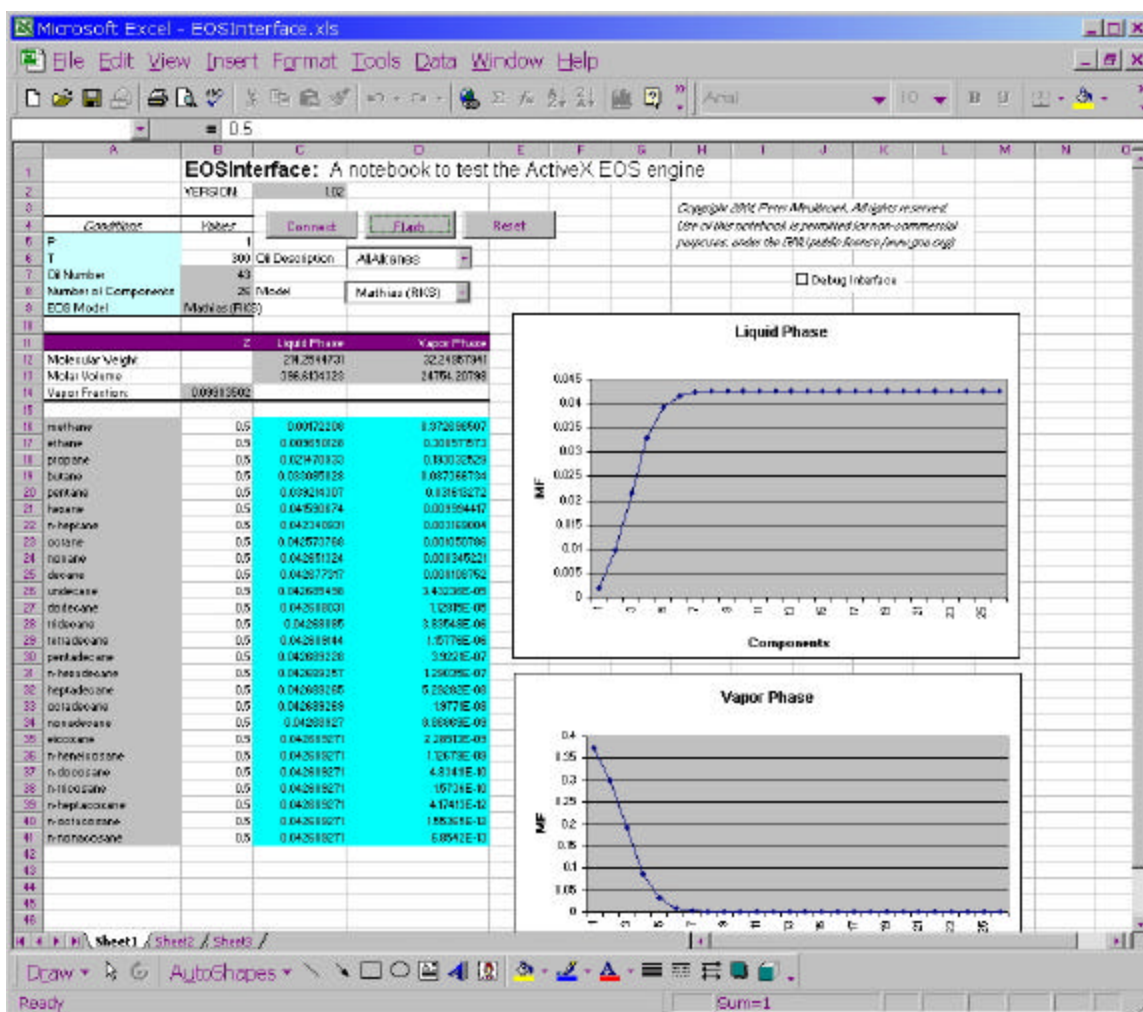
Figure 1: The Flash model prototype

As an aside, much of the installation work to combine the basin code with the flash code was done remotely using commercial collaboration software. Though still somewhat difficult to use, such software eliminated the need and expense of a trip between Caltech and Cornell.

Work has started on viscosity, diffusion constant, and surface-tension predicting routines to be bundled with the flash code. That work is expected to be complete by the end of the next reporting period.

TASK 4: CONVENTIONAL BASIN MODELING

Primary Responsibility	Subtask	Investigator
Cornell	2-D model	Cathles
Cornell	add maturity indicators	Cathles

Summary: The fourth task of the project is to "Build a conventional basin model and incorporate new maturity indicators and data bases in a user-friendly way". For the third year of the project, the sub-task is to "Test code, incorporate additional kinetic data bases, and write manuals".

This reporting period has seen the incorporation of the kinetic database developed over the life of the project in task 1 into the basin model. Other major developments include testing the flash model developed in Task 3. A new module was introduced last quarter to assess the cooling by rapid sedimentation. The topic is important but requires a whole-lithosphere model. To date, a test case with very encouraging results has been tested using a 100 km Louisiana Gulf of Mexico data set.

TASK 5: PRIMARY MIGRATION

Primary Responsibility	Subtask	Investigator
Cornell	2-D model	Cathles
Cornell	prototype algorithm	Cathles

Summary: The fifth task of the project is to "Develop an algorithm which combines the volume change and viscosities of the compositional maturation model to predict the chemistry of the hydrocarbons that will be expelled from the kerogen to the secondary migration pathways." For the third year, the subtask is to "establish necessary feedback chemical to finite difference flow model".

Work continues on the prototype primary migration algorithm developed by Yuling Zheng. The current reporting period has seen coupling between the physical model and transport model. This model has several significant bugs remaining, and hence requires further testing.

Further collaboration is planned during the next reporting period to address coupling the chemistry model produced under task 3 with the primary migration model.

TASK 6: SECONDARY MIGRATION

Primary Responsibility	Subtask	Investigator
Cornell	Develop prototype	Cathles

Summary: The sixth task of the project is to "Develop an algorithm that predicts the flow of hydrocarbons along secondary migration pathways, accounts for mixing of miscible hydrocarbon components along the pathway, and calculates the phase fractionation that will occur as the hydrocarbons move upward down the geothermal and fluid pressure gradients in the basin." The third year subtask is to "carry out test simulations to refine methods and debug". Future progress will require more functionality from the flash model produced in Task 3—in particular, the

prediction of viscosity and surface tension. The additional functionality should be available during the next reporting period.

TASK 7: INTEGRATION ON PC

Primary Responsibility	Subtask	Investigator
Geogroup	connect external code	Manhardt

Summary: The final task for the project is to "Integrate the above components into a functional model implemented on a PC or low cost workstation." For the third year, the subtask is to "Complete transfer from workstation to PC environment, and establish umbrella shell." Progress on this task has been substantial and regular. There have been three notable achievements:

1) Exporting plots. A big part of the utility of basin models comes from their ability to focus on a particular variable (such as temperature, hydrocarbon maturity, or pressure) as a function of time or location. Over the current reporting period, the ability to export plots, either as a stand-alone file or to the windows clipboard, has been added. While this ability is still in beta stage, it represents a big step in moving the model towards a usable product.

2) Communication framework. Progress continues on combining models from different tasks using the MS windows COM technology. This will provide extensibility to the basin model, and allow users to add their own routines.

3) Bug fixes. A major part of developing a new model is to find and fix the bugs that are inadvertently introduced into the code. Many such bugs have been found and squashed during this reporting period.